PARIS II: Computer Aided Solvent Design for Pollution Prevention

Abstract

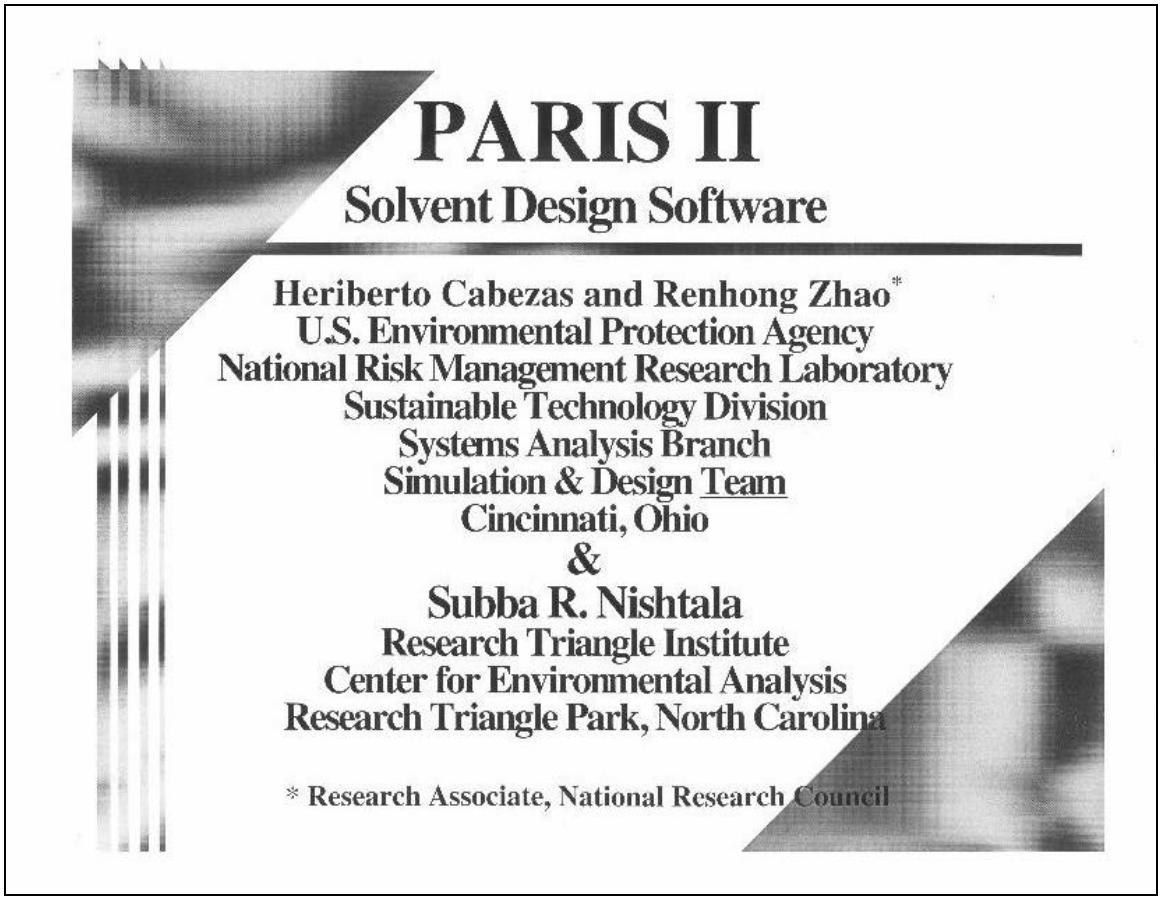
There is a great need to replace solvents currently used in industry but whose continued use presents a number of environmental difficulties. These difficulties include worker health concerns, environmental impacts such as ozone depletion, and toxicity in the environment. The replacement of these objectionable solvents, however, is rather a difficult task. One reason is that in order to successfully replace a solvent with another solvent or a solvent mixture, a great many solvent parameters and, for mixtures, different compositions need to be considered. The list of solvent parameters that need to be considered can include density, viscosity, surface tension, solvent capacity, etc., and can become quite large.

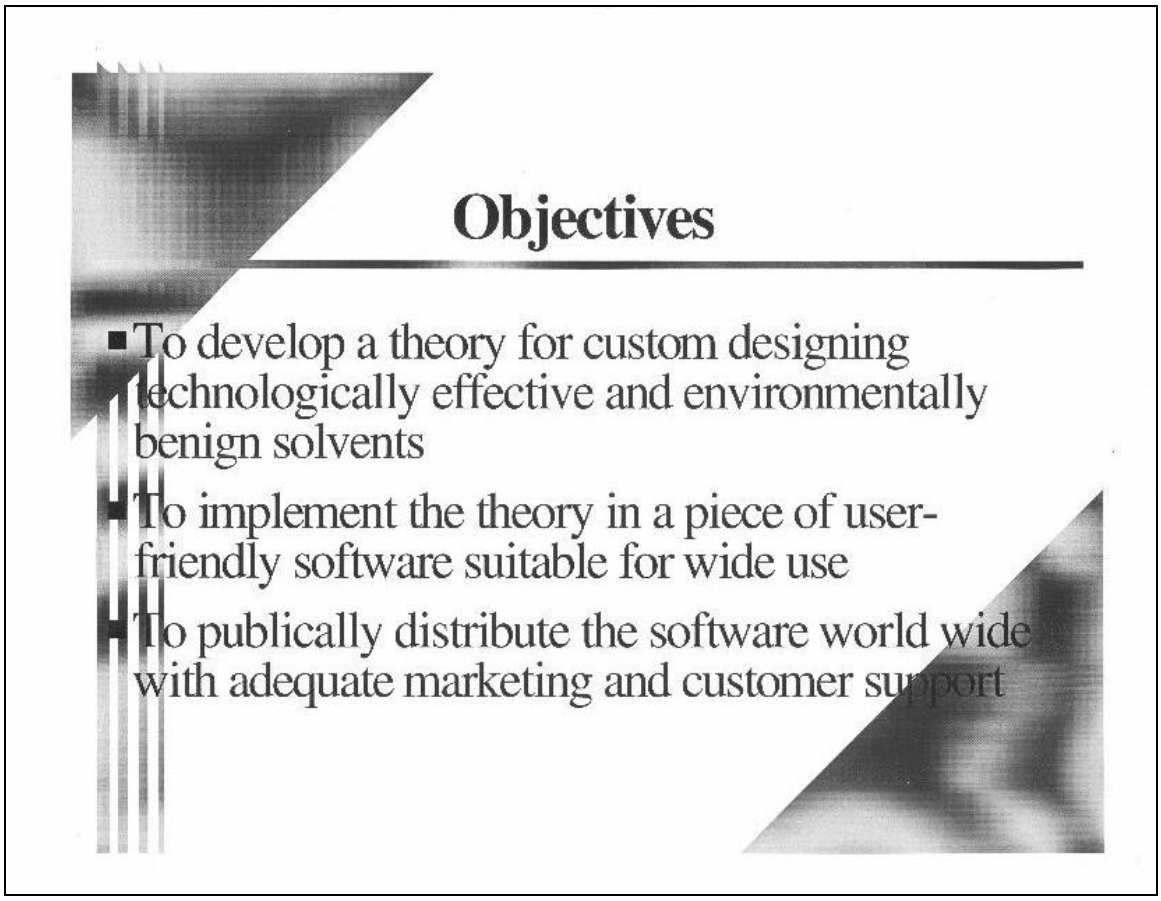
Clearly, trying to accomplish this replacement search by hand can become a nearly interminable task. It is also frequently desirable and more economical to replace only the solvent, but not the process or the equipment in which the solvent is being used. In order to replace only the solvent, it is further necessary to consider the various performance requirements for the solvent such as evaporation rate, flash point, etc. Including an appropriate set of solvent parameters and performance requirements in considering replacement solvents is extremely important to insure that the replacement will perform adequately.

At the US EPA's National Risk Management Research Laboratory, an effort is underway to develop a computer program that will allow users to design more benign replacement solvents. The software is entitled PARIS II which is am acronym for Program for Assisting the Replacement of Industrial Solvents, Version 2. The program is capable of going beyond solvent substitution into solvent design.

The solvent design capability allows the user to enhance desirable solvent properties while simultaneously suppressing undesirable ones such as, for example, toxicity. This is achieved by selecting appropriate mixtures of pure solvents and manipulating the composition. The composition is manipulated by a algorithm aided by a library of routines of fluid property prediction techniques and solvent performance requirements. The program contains a database of solvents, and lists of solvent properties and solvent performance requirements. The list of solvent properties adequately characterizes both the static and the dynamic behavior of the solvents. The list of solvent performance requirements includes comprehensive measures of toxicity and means to estimate volatile organic emissions among other items. The program develops a list of ranked candidate replacement pure solvents or solvent mixtures for consideration by the user.

Slide Presentation




Objectives
To develop a theory for custom designing technologically effective and environmentally benign solvents
To implement the theory in a piece of user-friendly software suitable for wide use
To publically distribute the software world wide with adequate marketing and customer support

Classification of Design Criteria

- Dynamic or Transport Properties
- Static or Equilibrium Properties
- Phase Stability Criteria
- Environmental Requirements
- Performance Requirements
- General Properties

Dynamic Properties

Isothermal Equation of Motion (x-component):

$$\rho\left(\frac{\partial v_x}{dt} + v_x\frac{\partial v_x}{\partial x} + v_y\frac{\partial v_x}{\partial y} + v_z\frac{\partial v_x}{\partial z}\right) = -\frac{\partial p}{\partial x} + \mu\left(\frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2} + \frac{\partial^2 v_x}{\partial z^2}\right) + \rho g_x$$

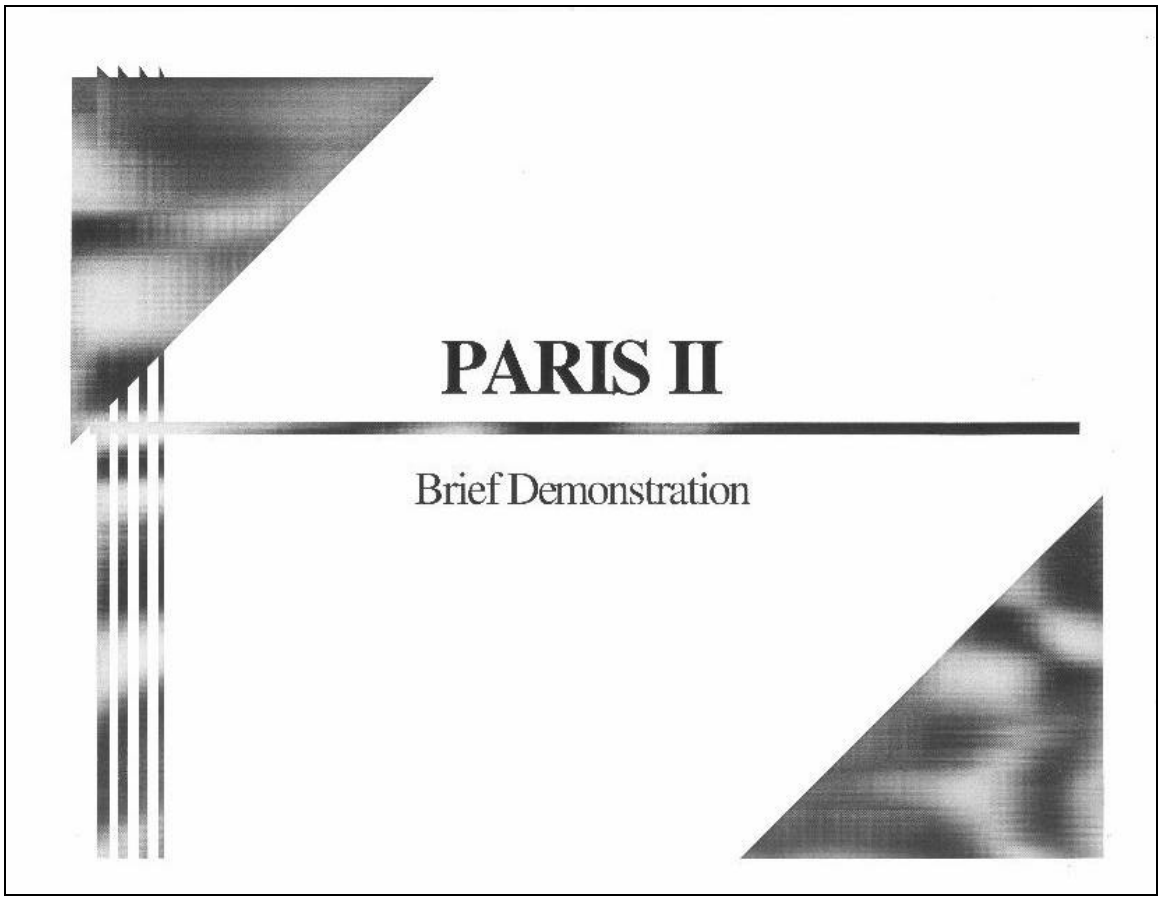
Dynamic Properties

The Three Modes of Transport

Newton's Law: $$\tau_{yx} = -\mu \frac{dv_x}{dy}$$

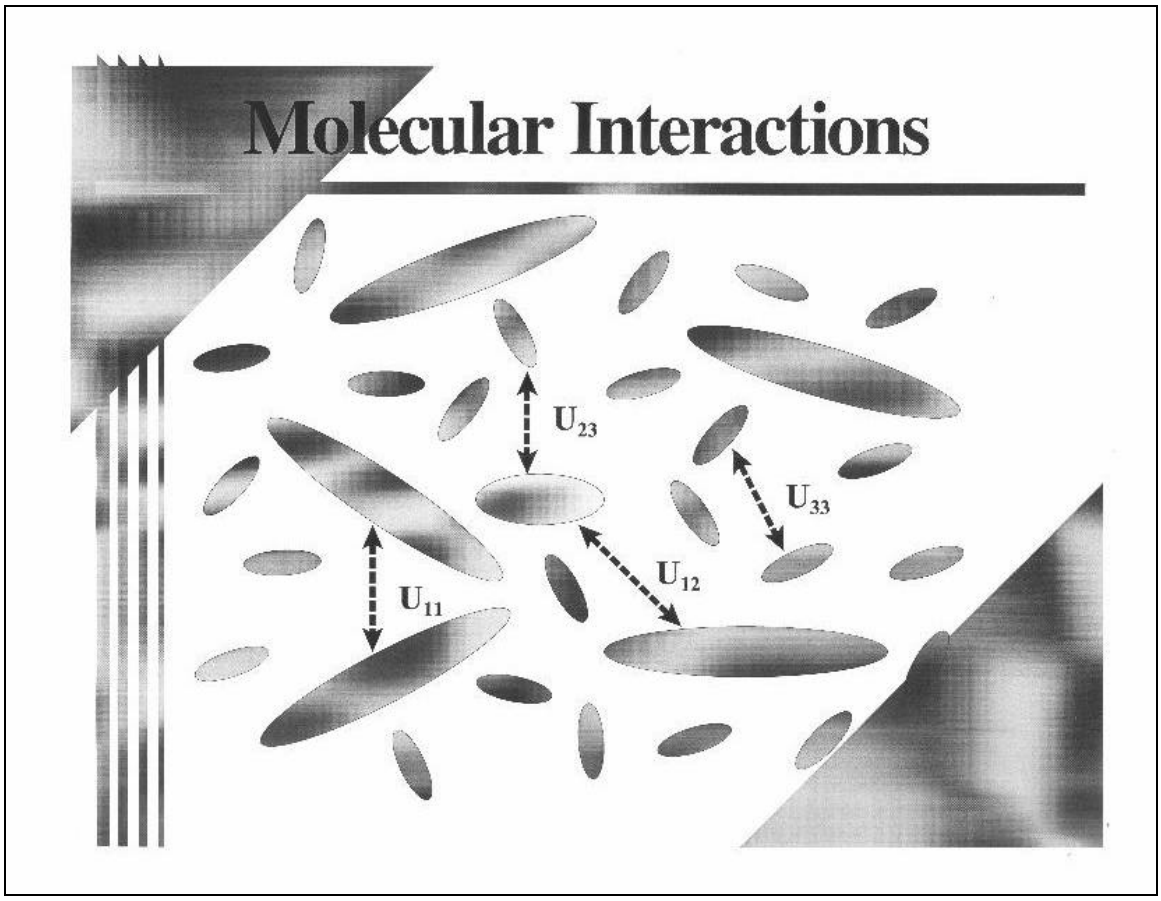
Fourier's Law: $$q_y = -\kappa \frac{dT}{dy}$$

Fick's Law: $$J_{Ay} = -D_{AM} \frac{dC_A}{dy}$$


PARIS II
Brief Demonstration

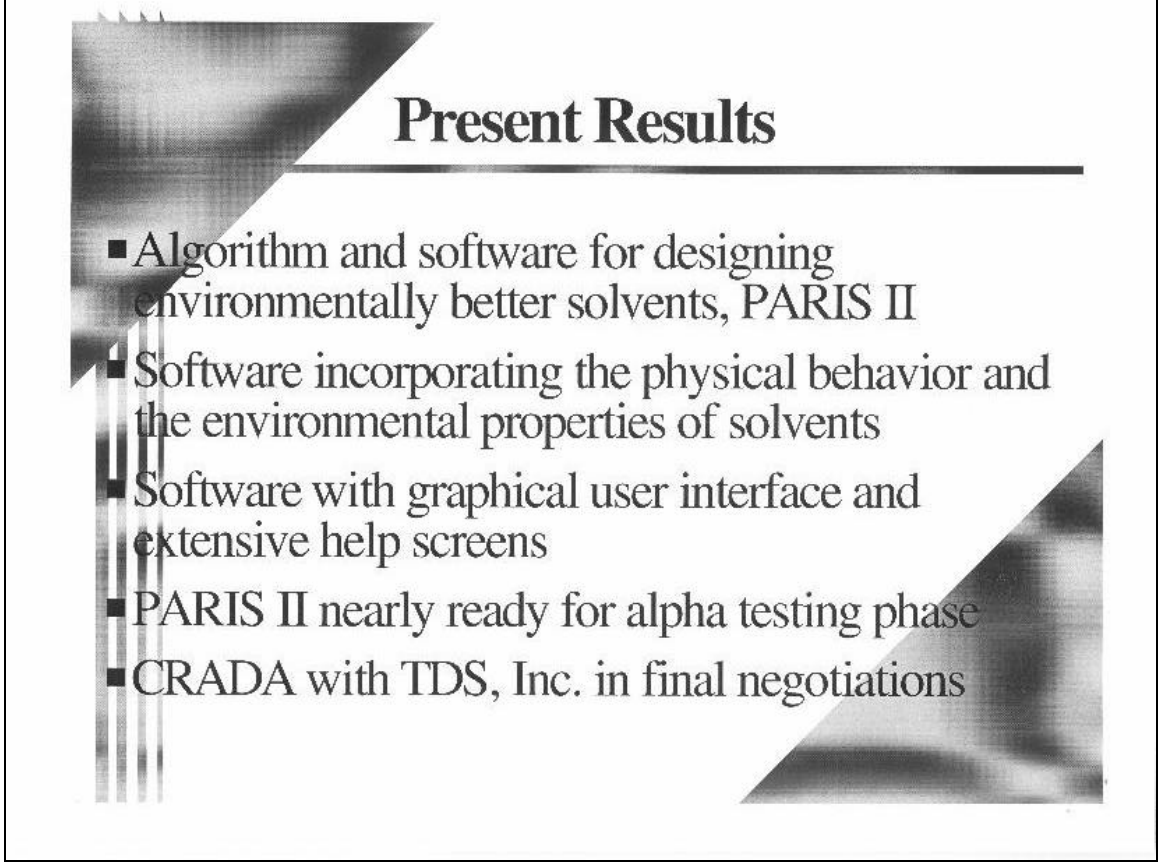
Physical Properties of Solvents

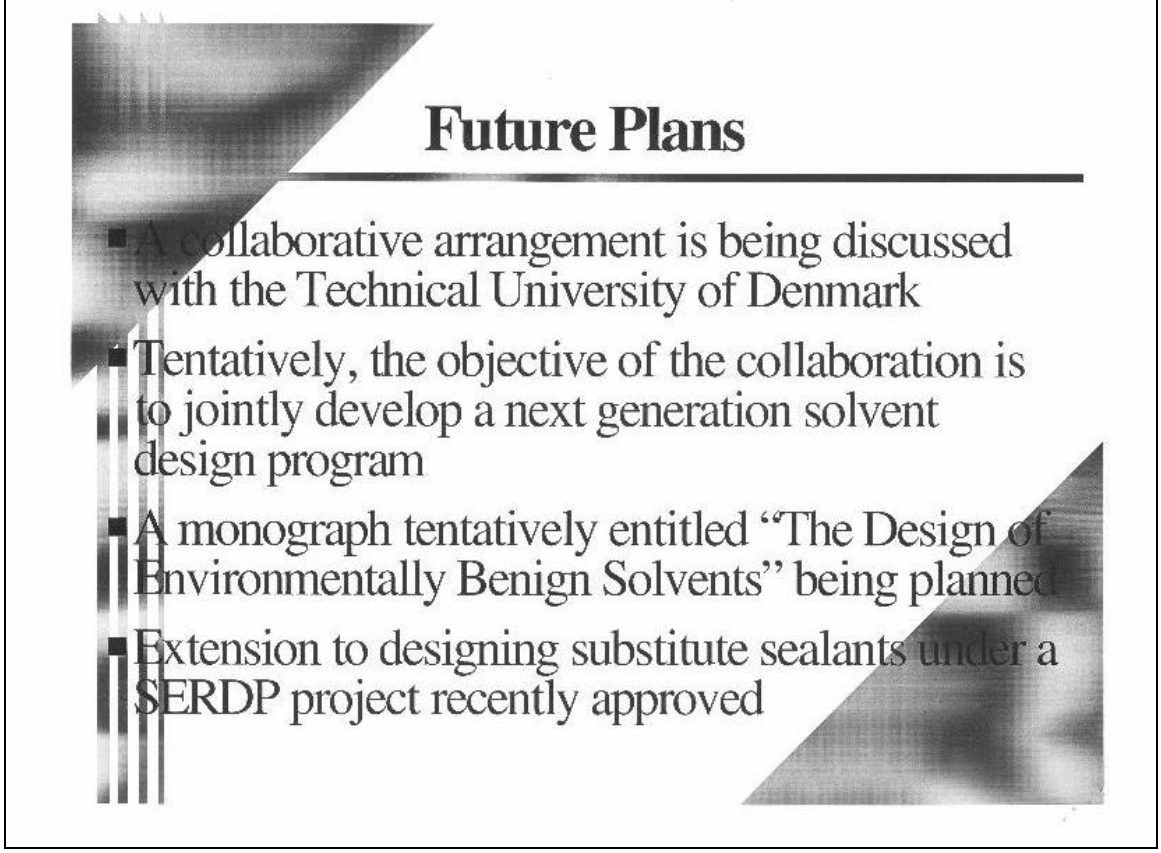
	Benzene	Cyclohexene	Toluene
Molecular Mass (kg/kmole)	78.114	82.145	92.141
MolarVolume (m^3/kmole)	0.0895	0.1019	0.1066
Boiling Temperature (K)	353.24	356.12	383.78
Vapor Pressure (kPa)	12.659	11.823	3.793
Surface Tension (N/m)	0.0282	0.0261	0.0279
Viscosity x10^4 (N- s/m^2)	6.009	6.180	5.548
Thermal Conduct. (W/m-K)	0.138	0.130	0.133
Flash Point (K)	262.04	266.48	277.59


Molecular Interactions
U_{23}
U_{33}
U_{12}
U_{11}

γ_i^{∞}, Infinite Dilution Activity Coefficients

	Benzene	Cyclohexene	Toluene
Ethanol	10.2	26.6	11.3
Diethyl Ether	0.97	1.2	1.1
Acetone	1.5	4.7	1.9
Water	1770	369	2700
Octanol	2.2	0.95	2.5
Benzene	N/A	1.3	1.0


Present Results
Algorithm and software for designing environmentally better solvents, PARIS II
Software incorporating the physical behavior and the environmental properties of solvents
Software with graphical user interface and extensive help screens
PARIS II nearly ready for alpha testing phase
CRADA with TDS, Inc. in final negotiations


Future Plans
A collaborative arrangement is being discussed with the Technical University of Denmark
Tentatively, the objective of the collaboration is to jointly develop a next generation solvent design program
A monograph tentatively entitled "The Design of Environmentally Benign Solvents" being planned
Extension to designing substitute sealants under a SERDP project recently approved